wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 11:29 PM EDT

PDB ID	:	3LOG
Title	:	Crystal structure of MbtI from Mycobacterium tuberculosis
Authors	:	Bulloch, E.M.M.; Lott, J.S.; Baker, E.N.; Johnston, J.M.
Deposited on	:	2010-02-03
Resolution	:	1.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

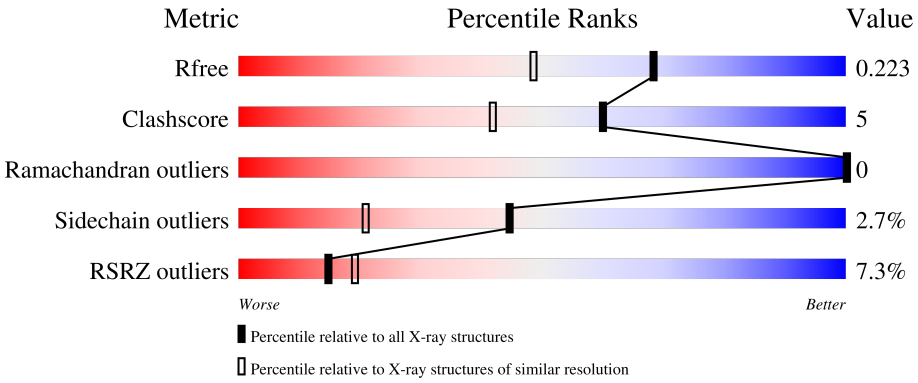
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	4% 86% 10%
1	B	451	4% 90% 9%
1	C	451	3% 86% 9%
1	D	451	17% 89% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	451	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

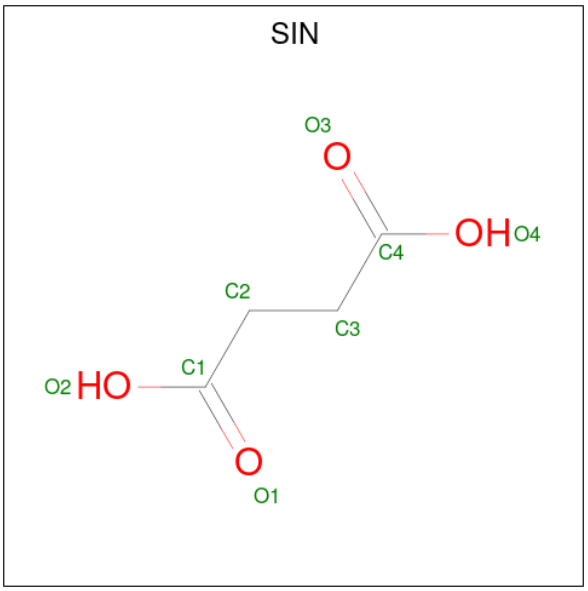
- Molecule 1 is a protein called Isochorismate synthase/isochorismate-pyruvate lyase mbtI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	11	0
			3381	2117	616	637	11			
1	B	450	Total	C	N	O	S	0	10	0
			3481	2174	636	660	11			
1	C	435	Total	C	N	O	S	0	9	0
			3366	2111	611	634	10			
1	D	440	Total	C	N	O	S	0	6	0
			3386	2117	617	642	10			

There are 8 discrepancies between the modelled and reference sequences:

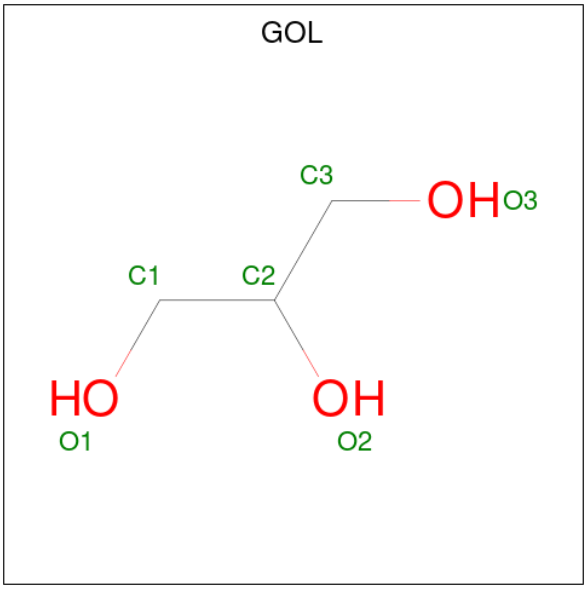
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q7D785
A	0	SER	-	expression tag	UNP Q7D785
B	-1	GLY	-	expression tag	UNP Q7D785
B	0	SER	-	expression tag	UNP Q7D785
C	-1	GLY	-	expression tag	UNP Q7D785
C	0	SER	-	expression tag	UNP Q7D785
D	-1	GLY	-	expression tag	UNP Q7D785
D	0	SER	-	expression tag	UNP Q7D785

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 4 4	0	0
2	A	1	Total C O 8 4 4	0	0
2	B	1	Total C O 8 4 4	0	0
2	C	1	Total C O 8 4 4	0	0
2	D	1	Total C O 8 4 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

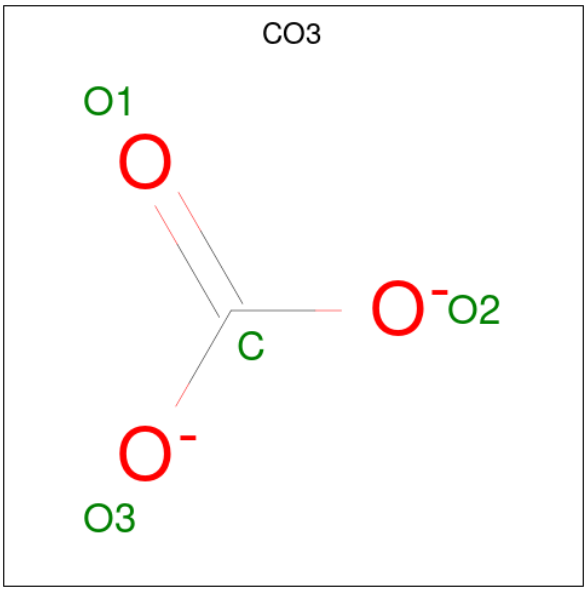


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 1 3	0	0

- Molecule 6 is water.

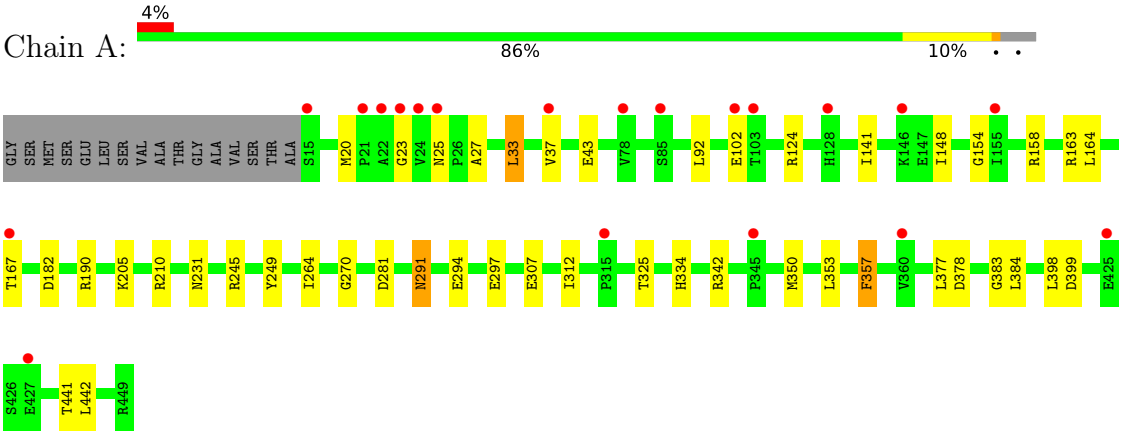
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	413	Total O 413 413	0	0
6	B	448	Total O 448 448	0	0
6	C	455	Total O 455 455	0	0
6	D	308	Total O 308 308	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

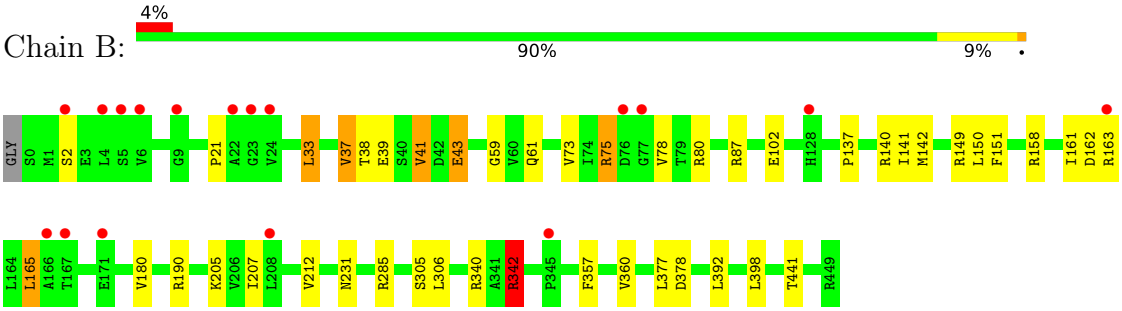
• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain A:



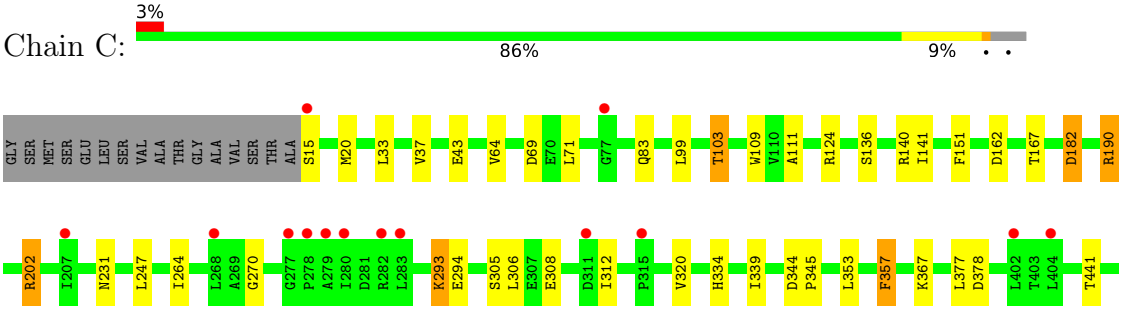
• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain B:



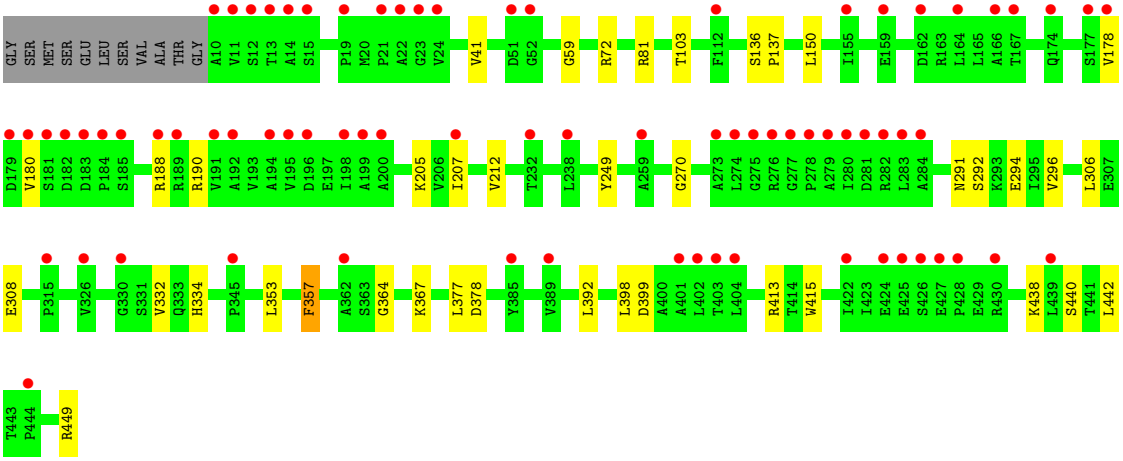
• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain C:



• Molecule 1: Isochorismate synthase/isochorismate-pyruvate lyase mbtI

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.87Å 115.70Å 93.89Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	50.00 – 1.73 28.80 – 1.73	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-1.73) 96.8 (28.80-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.73Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.225 0.179 , 0.223	Depositor DCC
R_{free} test set	9542 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15313	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CO3, GOL, SIN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.83	1/3469 (0.0%)	0.85	5/4708 (0.1%)
1	B	0.84	1/3569 (0.0%)	0.85	5/4841 (0.1%)
1	C	0.80	0/3451	0.84	6/4685 (0.1%)
1	D	0.76	0/3462	0.78	0/4702
All	All	0.81	2/13951 (0.0%)	0.83	16/18936 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	GLU	CG-CD	5.82	1.60	1.51
1	A	307	GLU	CG-CD	5.04	1.59	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	ARG	NE-CZ-NH2	-11.51	114.55	120.30
1	B	87	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	C	124	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	C	20	MET	CG-SD-CE	-7.04	88.94	100.20
1	C	69	ASP	CB-CG-OD1	5.81	123.53	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3381	0	3413	32	0
1	B	3481	0	3520	34	0
1	C	3366	0	3397	28	0
1	D	3386	0	3406	31	0
2	A	16	0	8	3	0
2	B	8	0	4	0	0
2	C	8	0	4	0	0
2	D	8	0	4	1	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
3	D	6	0	7	6	0
4	B	1	0	0	0	0
5	B	4	0	0	0	0
6	A	413	0	0	5	0
6	B	448	0	0	6	0
6	C	455	0	0	5	0
6	D	308	0	0	2	0
All	All	15313	0	13795	126	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 126 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340[B]:ARG:HG2	1:B:340[B]:ARG:HH11	0.95	1.11
1:B:340[B]:ARG:HG2	1:B:340[B]:ARG:NH1	1.73	0.95
1:D:415:TRP:CZ2	3:D:451:GOL:H11	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:TRP:HZ2	3:D:451:GOL:H11	1.39	0.88
1:B:140[B]:ARG:NH1	6:B:1043:HOH:O	2.04	0.88

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/451 (98%)	438 (99%)	6 (1%)	0	100	100
1	B	458/451 (102%)	453 (99%)	5 (1%)	0	100	100
1	C	442/451 (98%)	437 (99%)	5 (1%)	0	100	100
1	D	444/451 (98%)	440 (99%)	4 (1%)	0	100	100
All	All	1788/1804 (99%)	1768 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/358 (99%)	349 (98%)	7 (2%)	55	33
1	B	367/358 (102%)	352 (96%)	15 (4%)	30	9
1	C	353/358 (99%)	345 (98%)	8 (2%)	50	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	355/358 (99%)	346 (98%)	9 (2%)	47 24
All	All	1431/1432 (100%)	1392 (97%)	39 (3%)	44 21

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	357	PHE
1	D	413	ARG
1	C	378	ASP
1	D	332	VAL
1	D	440[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	61	GLN
1	D	291	ASN
1	C	25	ASN
1	C	83	GLN
1	C	231	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CO3	B	452	4	2,3,3	0.61	0	2,3,3	2.05	1 (50%)
2	SIN	D	450	-	7,7,7	1.15	0	8,8,8	1.57	3 (37%)
3	GOL	C	451	-	5,5,5	0.43	0	5,5,5	0.73	0
2	SIN	B	450	-	7,7,7	1.04	0	8,8,8	1.57	1 (12%)
3	GOL	A	452	-	5,5,5	0.39	0	5,5,5	0.52	0
2	SIN	A	450	-	7,7,7	1.12	0	8,8,8	1.53	2 (25%)
3	GOL	D	451	-	5,5,5	1.13	1 (20%)	5,5,5	1.12	0
2	SIN	C	450	-	7,7,7	0.87	0	8,8,8	2.75	2 (25%)
3	GOL	B	453	-	5,5,5	0.64	0	5,5,5	0.95	0
3	GOL	C	452	-	5,5,5	0.35	0	5,5,5	0.48	0
2	SIN	A	451	-	7,7,7	0.95	0	8,8,8	2.49	4 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIN	D	450	-	-	2/5/5/5	-
3	GOL	C	451	-	-	0/4/4/4	-
2	SIN	B	450	-	-	2/5/5/5	-
3	GOL	A	452	-	-	2/4/4/4	-
2	SIN	A	450	-	-	2/5/5/5	-
3	GOL	D	451	-	-	0/4/4/4	-
2	SIN	C	450	-	-	2/5/5/5	-
3	GOL	B	453	-	-	2/4/4/4	-
3	GOL	C	452	-	-	2/4/4/4	-
2	SIN	A	451	-	-	3/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	451	GOL	O2-C2	-2.29	1.36	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	450	SIN	C2-C3-C4	-6.70	99.18	113.60
2	A	451	SIN	C3-C2-C1	-4.97	102.90	113.60
2	A	451	SIN	O2-C1-O1	-2.71	116.55	123.30
2	A	450	SIN	O2-C1-C2	2.61	122.41	114.03
2	C	450	SIN	O4-C4-O3	-2.52	117.02	123.30

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	452	GOL	O1-C1-C2-C3
3	C	452	GOL	O1-C1-C2-C3
2	A	451	SIN	C1-C2-C3-C4
3	B	453	GOL	C1-C2-C3-O3
3	C	452	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	450	SIN	1	0
3	A	452	GOL	1	0
3	D	451	GOL	6	0
2	A	451	SIN	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	435/451 (96%)	0.36	20 (4%)	32	38	23, 32, 54, 71	0
1	B	450/451 (99%)	0.25	17 (3%)	40	46	21, 30, 49, 59	0
1	C	435/451 (96%)	0.14	15 (3%)	45	51	22, 31, 44, 56	0
1	D	440/451 (97%)	0.81	76 (17%)	1	2	24, 38, 57, 63	0
All	All	1760/1804 (97%)	0.39	128 (7%)	15	19	21, 32, 52, 71	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	279	ALA	7.6
1	B	6	VAL	7.2
1	A	22	ALA	6.2
1	A	23	GLY	6.1
1	D	278	PRO	5.9

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SIN	A	451	8/8	0.73	0.21	37,51,58,63	0
3	GOL	B	453	6/6	0.81	0.20	37,40,44,52	0
3	GOL	A	452	6/6	0.83	0.14	51,60,61,63	0
3	GOL	D	451	6/6	0.85	0.17	41,52,55,56	0
3	GOL	C	452	6/6	0.86	0.20	41,51,56,56	0
2	SIN	C	450	8/8	0.87	0.20	29,39,61,62	0
5	CO3	B	452	4/4	0.88	0.15	41,43,46,46	0
2	SIN	D	450	8/8	0.90	0.22	38,47,56,57	0
3	GOL	C	451	6/6	0.93	0.09	36,39,46,52	0
2	SIN	B	450	8/8	0.95	0.18	25,33,47,52	0
4	NA	B	451	1/1	0.97	0.14	36,36,36,36	0
2	SIN	A	450	8/8	0.97	0.11	26,31,41,45	0

6.5 Other polymers (i)

There are no such residues in this entry.